

Paramagnetism of the oxygen molecule and the three-electron bond.

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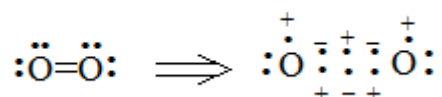
The oxygen molecule is paramagnetic and, what is important, has a bond multiplicity equal to 2 (this is an experimental fact, IR spectra).

Therefore, it is impossible to adequately represent the oxygen formula in the classical language of chemistry, i.e. Lewis formulas. But the distribution of electron density in the molecule must be stationary and averaged over time, therefore, the structure of the oxygen molecule can still be conveyed by the formula.

It is necessary to realize the simple fact that the oxygen formula cannot be written down unless we accept that there is a real three-electron bond with a normal multiplicity, i.e. 1.5.

Then, the oxygen molecule can be correctly represented using two three-electron bonds and two unpaired electrons on oxygen atoms. But, according to the octet rule, each oxygen atom must have an octet of 8 electrons. Therefore, some of the bond electrons will not be taken into account (we do not take into account 1 electron; or more precisely, two half-electrons), which means that the unpaired electrons located on the oxygen atoms actively interact with the bond electrons, which leads to a decrease in multiplicity.

Only in this way can the formula of the oxygen molecule be adequately depicted, since the molecule is paramagnetic and has a bond multiplicity of 2. Here is the formula [1].



In conclusion, I will note that the theory of molecular orbitals, which for the first time adequately explained the paramagnetism of the oxygen molecule, is in insurmountable contradiction with the principle of quantum superposition - the principle of quantum superposition prohibits obtaining MOs whose energy level differs from the original AOs.

Principle of quantum superposition [2]:

“...Suppose that in a state with a wave function $\psi_1(q)$ some measurement leads with certainty to a certain result - result 1, and in a state $\psi_2(q)$ - to result 2. Then it is assumed that any function of the form $C_1\psi_1 + C_2\psi_2$ (C_1, C_2 - constants), describes a state in which the same measurement will give either result 1 or result 2...

These statements constitute the content of the so-called principle of superposition of states - the main positive principle of quantum mechanics. It follows from it, in particular, that all equations satisfied by the wave functions must be linear in ψ ...”.

1. Bezverkhniy V. D. Structure of the Benzene Molecule on the Basis of the Three-Electron Bond. SSRN Electronic Journal, Nov 2017. P. 28. <https://dx.doi.org/10.2139/ssrn.3065241>
2. Landau L. D., Lifshits E. M. Theoretical physics in 10 volumes. Volume 3. Quantum mechanics. Fourth edition. Moscow, Nauka, 1989, pp. 20 - 21.